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Charliecloud

Unprivileged Containers for User-Defined Software Stacks in HPC

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Los Alamos National Laboratory

- Established in 1943 as “Site Y” of the Manhattan Project to create atomic bomb
- Mission: To solve National Security challenges through Scientific Excellence
- Part of the NNSA “Tri-Lab” partnership with Lawrence Livermore and Sandia Labs
- We perform a wide variety of classified and open scientific research and development.
- Funded primarily by the Department of Energy, we also do extensive work for/with the Departments of Defense and Homeland Security, the Intelligence Community, et al.
- Our strategy reflects US government priorities including nuclear security, intelligence, defense, emergency response, nonproliferation, counterterrorism, and more.
- We help to ensure the safety, security, and effectiveness of the US nuclear stockpile.
- Since 1992, the United States no longer performs full-scale testing of nuclear weapons. This has necessitated continuous, ongoing leadership in large-scale simulation capabilities realized through investment in high-performance computing.

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LANL HPC Division

- LANL's history in high-performance computing is long and storied, dating back to the early '50s.
- Accomplishments include:
  - Helped IBM develop the 1st transistor-based supercomputer, Stretch
  - Our CM-5 was #1 on the inaugural Top500 List
  - The 1st vector computer, Cray-1, deployed here
  - 1st hybrid supercomputer (using IBM POWER and PlayStation Cell processors), Roadrunner, was also 1st to break the PetaFLOP/s barrier
- Led by Gary Grider, creator of Burst Buffer technology

- We support over 2000 unique users across more than 100 different classified/open science projects on 20+ clusters

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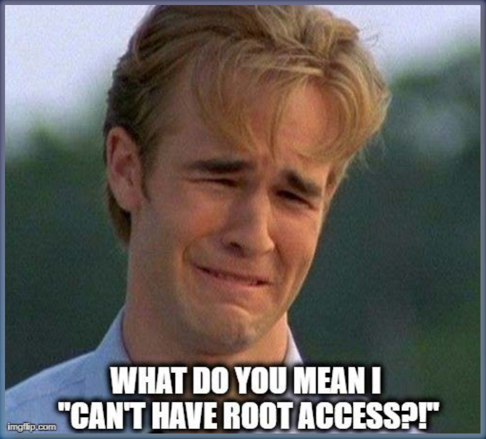
First World Problems in HPC



Problem #1: HPC clusters have narrowly focused software stacks.

- They do serial and parallel-MPI tasks well...but that's it.
- Compute node images are often in RAM/NFS & kept small.
- Managing multiple OSs, and required expertise, is rare & labor intensive.

Problem #2: We're old. And not getting any younger.

- Schools are teaching clusters, "parallel"/scalable/distributed software development...but usually "embarrassingly parallel" (e.g., map/reduce)
- All the "cool kids" are using Ubuntu (or Arch, or Alpine...), not RHEL
- Modern Machine Learning and Data Analytics toolsuites are non-trivial

Problem #3: We are finite, as is our time.

- We generally won't install extra software with low user demand.
- Unique or unusual use cases tend to be lower priority.
- The line between "innovator" and "crackpot" is often rather blurry….

The Solution: UDSS/UDI/BYOE

User-Defined Software Stacks (UDSS) allow users to supply not only their own applications/source to run on HPC systems but also the environment -- up to and including entire OS images -- in which they should run!

Advantages include portability, usability, consistency, time savings…

Potential disadvantages include missing functionality (HSN, accelerators, filesystems), performance degradation; thus, addressing these should be part of the design of any HPC-focused solution!

In rare, specific cases, certain packages may address this independently by building static binaries or otherwise coupling dependencies with executables

- Works everywhere
- No privileges required
- Requires build-time support
- May or may not be feasible
- For everyone else, our options are...

Option #1: Compile It Yourself

Advantages

- Available everywhere immediately
- Requires no privileges
- No additional privacy/security risk
- Direct access to all hardware
- No performance penalty
- Theoretically applies to any open source software library/app/stack

Disadvantages

- ...but it’s, like, 2017. And stuff.
- Tedious and time-consuming
- Error-prone
- Hard to update
- No standard workflow
- Provides neither portability nor consistency

Nope.

Option #2: Environment Manager

Advantages
- Available for most IA32/x64 systems
- Requires no privileges
- No additional privacy/security risk
- Direct access to all hardware
- No performance penalty

Disadvantages
- Frequently still requires building from source (time/space constraints)
- Varying degrees of HPC support
- Varying degrees of reproducibility, portability, consistency, workflow
- Users/consultants bear entire burden

If You Must…
- Good options include EasyBuild, Lmod, Spack
- Also Anaconda, nixOS

"There's GOT to be a BETTER WAY!!"

Option #3: Virtualization (VMs)

Advantages
- Ultra-flexible (any kernel/OS/arch)
- Strong-to-complete isolation
- Common use cases perform well

Disadvantages
- Performance suffers for most HPC use cases, often significantly
- Performance/isolation tradeoffs
- Infrastructure can be complex
- Direct/performant access to hardware may require privileges
- Not all “exotic” HPC hardware supported
- Entire OS must be provisioned and booted, separate hostname/IP, etc.

Should HPC become the Cloud?

Option #4: Containers

Advantages

- Enough flexibility (only share kernel)
- Enough isolation (namespaces, etc.)
- Standard, reproducible workflow
- Bare-metal performance (or close)
- Minimal or no user/consultant burden (presumes correct solution choice)
- Extremely simple and easy-to-use (presumes correct solution choice)

Disadvantages

- Require recent Linux kernel/distro (SLES 12SP2, RHEL 7.4, Ubuntu 16.04, Linux LTS 4.4/4.9) ***or*** privilege
- Occasional growing pains due to newness (feature-complete in 2013)
- Container expertise in HPC still rare; thus, bad info/myths are pervasive!

Should HPC use containers?

So...Umm...These Container Things...Like, What Are They?

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Good question! Not everyone agrees. Here's our take.

Linux Containers:

- Use one or more kernel ***namespaces*** to provide isolation for (i.e., "contain") a process (along with its child processes, if any);
- Envelope/restrict the process(es) such that escape/escalation is "impossible;" and
- Facilitate application security by providing capability constraints, integrity assurance, and content validation via industry-standard formats and workflows.

Namespaces, You Say?

The Linux Kernel supports 6 namespaces as of version 3.8, 7 as of 4.6.

- 6 Privileged Namespaces (require `CAP_SYS_ADMIN` to create)
  - `mount` – Private filesystem mount points, recursion/propagation controls
  - `pid` – Private view of process IDs and processes, `init` semantics
  - `uts` – Private hostname and domainname values
  - `net` – Private network resources (devices, IPs, routes, ports, etc.)
  - `ipc` – Private IPC resources (SysV IPC objects, POSIX msg queues)
  - `cgroup` – Private control group hierarchy (Linux 4.6+ only)
- 1 Unprivileged Namespace (requires no special capabilities to create)
  - `user` – Private UID and GID mappings
    - Can be combined with other namespaces, even if unprivileged
- System Call API: `unshare(2)`, `clone(2)`, `setns(2)`

Further reading: "Namespaces in Operation" (https://lwn.net/Articles/531114/)

The Container Landscape

Full-featured Container Systems

- Support building, distribution, validation, and execution
- Provide for complete handling of containers throughout lifecycle
- Examples: Docker, Rocket, LXC/LXD
- Most modern container engines now implement Open Container Initiative (OCI) Image and/or Runtime Specification(s)
- Building containers is still a per-system function. OCI does NOT do building!
  - `Dockerfiles` are the de facto standard; robust, capable DSL
  - CoreOS Rocket supplied `acbuild` based around traditional shell-fu

Lightweight Container Systems

- Generally only provide runtime; most leverage Docker ecosystem
- Tend to require existing directory tree (i.e., flattened image) to run in
- Examples: RunC, CCon, NsJail, `unshare(1)`, `systemd-nspawn(1)`
- …and of course, Charliecloud!

Additional Container Elements

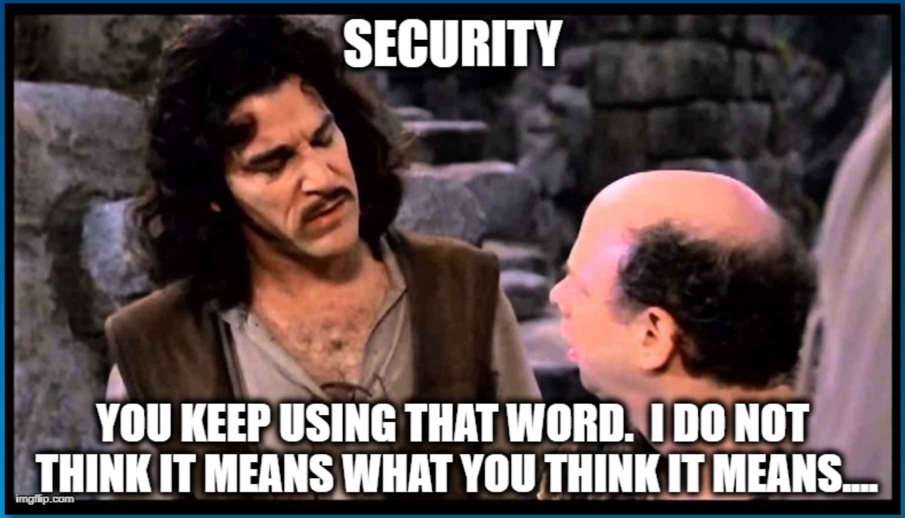
The Linux kernel has several additional subsystems that containers use:

- `cgroups` – Control hierarchical resource management and constraint
  - Latest kernels (4.6+) even have namespaces for this!
  - This is how modern schedulers/RMs track/control job resource usage
- `seccomp-bpf` – Berkeley Packet Filter-based system call filtering
  - Frequently used to prevent containers exceeding their scope
- `prctl(PR_SET_NO_NEW_PRIVS)` – Prevent privilege escalation
  - Permanent, kernel-level flag that prevents `execve()` ever granting privileges
  - Preserved across all calls to `fork()`, `clone()`, and `execve()`
- SELinux – Labeling system for filesystems and applications
  - Allows admins precise control over actions, roles of applications
- AppArmor – Profile-based MAC system for limiting applications' abilities
  - Similar to SELinux but without filesystem labeling features

Let's Talk Security

As with all aspects of Cybersecurity, true security isn't merely the absence of access but rather the presence of protection!

- Container security relies entirely on the separation of authorities which exists inside the Linux kernel. If the kernel fails, the container fails.
- Container security relies, among other things, on a wide variety of content assurance methodologies (e.g., non-repudiation, CAS) along with aforementioned protections.
- Lightweight container solutions have the advantage of leaving much of that to others.



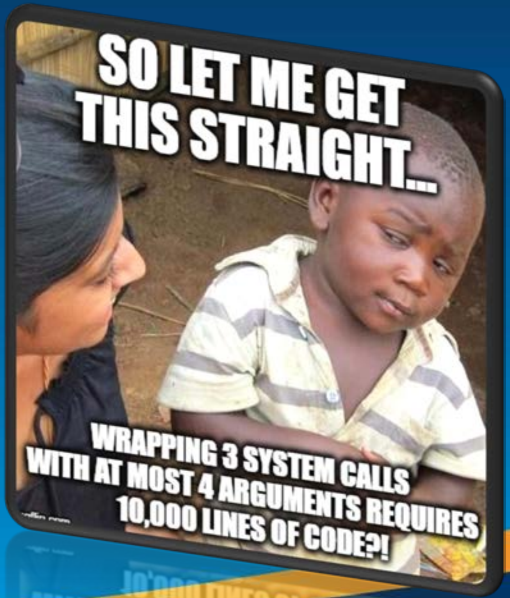
Question: Is Docker "Insecure?"

Short Answer: Nope.

Longer Answer: Absolutely, positively, without a doubt…nope. Not any more. Ignore the FUD.

Why Charliecloud?

- Docker has a great security story (now) but not a great performance story!
  - OverlayFS is slooooooow due to layering
  - File removal is done literally by “whiting out”
  - Subtle nuances with, e.g., Yum/RPMDB
  - Charliecloud leverages OCI-like “flattened” directory structure
- HPC users don’t need flexibility/overhead of `config.json`
  - Inside user namespace, other namespaces can be created/joined using `unshare(1)`, `nsenter(1)`
  - Additional security hardening coming soon
- A simple API should result in small, simple code
  - Charliecloud weighs in at fewer than 1000 LoC
  - Compare to NSJail (4,000), Shifter (19,000), Singularity (14,000), and Docker (133,000)!

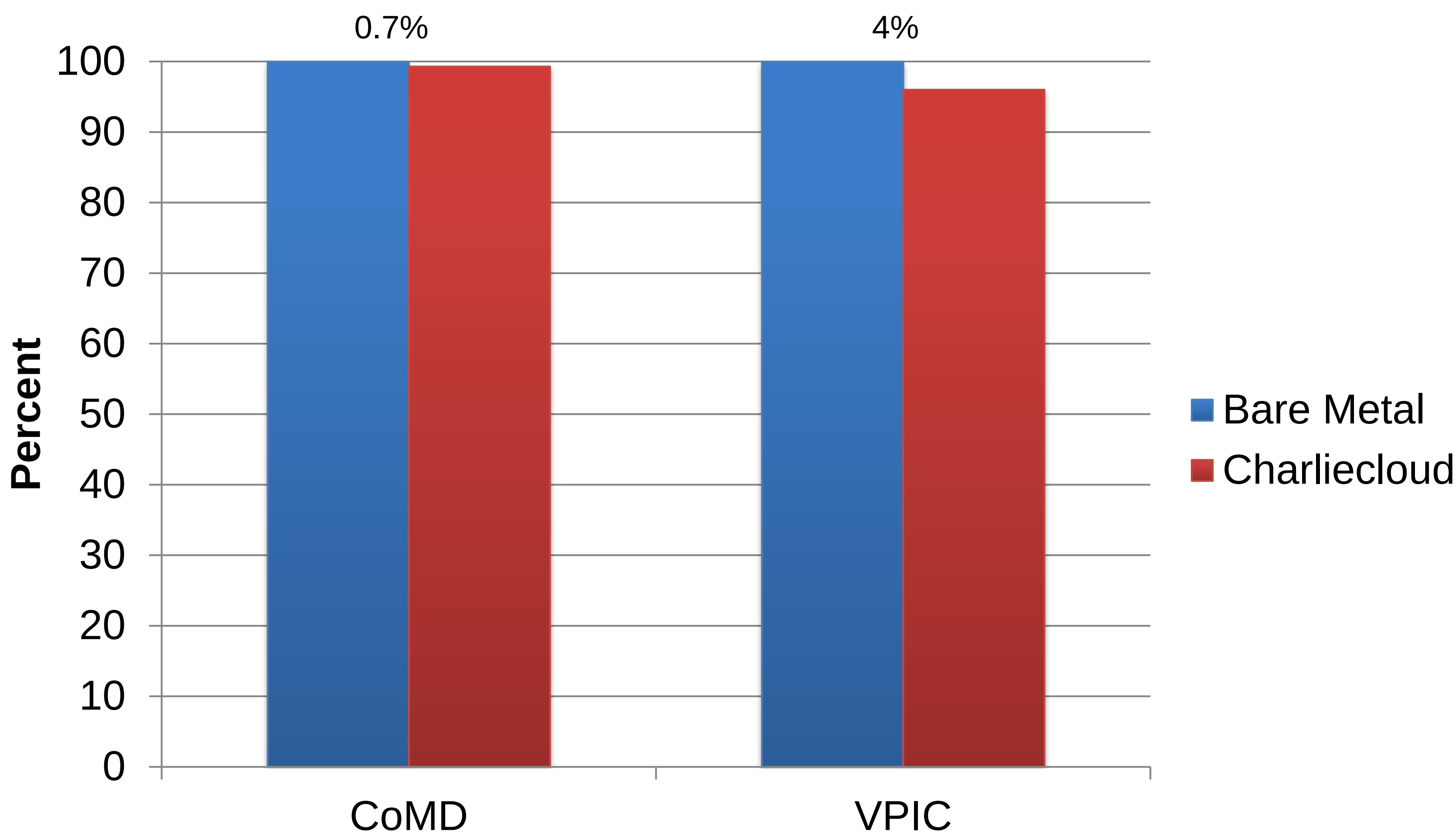


Charliecloud Demo/Walkthrough

```
$ cd ~/charliecloud/examples/serial/hello
$ ls
Dockerfile  hello.sh  README  test.bats
$ ch-build -t hello ~/charliecloud
Sending build context to Docker daemon 15.19 MB
[...]
Successfully built 30662b3f94f3
$ ch-docker2tar hello /var/tmp
57M /var/tmp/hello.tar.gz
```

```
$ ch-tar2dir /var/tmp/hello.tar.gz /var/tmp/hello
creating new image /var/tmp/hello
/var/tmp/hello unpacked ok
$ ch-run /var/tmp/hello -- cat /etc/debian_version
8.9
```

Charliecloud MPI Performance



Charliecloud Resources

- Supercomputing 2017 Paper
  by Reid Priedhorsky and Tim Randles
  - “Charliecloud: Unprivileged Containers for UDSS in HPC”
  - Los Alamos Tech Report LA-UR-16-22730
  - http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-16-22370
- ;login: Article “Linux Containers for Fun & Profit in HPC”
  by Reid Priedhorsky
  - https://www.usenix.org/publications/login/fall2017/priedhorsky
- Documentation: https://hpc.github.io/charliecloud (includes tutorials!)
- Source Code: https://github.com/hpc/charliecloud
- Mailing List: charliecloud@groups.io || https://groups.io/charliecloud
- Contact Reid (reidpr@lanl.gov), Tim (trandles@lanl.gov),
  or Michael (mej@lanl.gov, @mej0 on Twitter)

Questions/Comments?

THANK YOU!

PS: These slides, and all unclassified LANL publications, are available via LA-UR number at:
http://permalink.lanl.gov/object/tr?what=info:lanl-repo/lareport/LA-UR-17-29797